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13. ABSTRACT (Maximum 200 words)

We developed mathematical models for problems involving the fabrication of ceramic-matrix composites, the coating of ceramic fibers, and the oxidation of ceramic-matrix composites. To solve these models, we developed an adaptive and parallel computational framework for the finite element and finite volume solution of partial differential equations. The parallel adaptive framework handles mesh generation, refinement, and coarsening; dynamic load balancing; distributed database management; interprocessor communications; data migration; time integration; and algebraic solutions. The models and solutions revealed improved processing techniques for a reactive vapor infiltration application and potentially superior strategies for coating fibers. Oxidation studies are investigating the "self healing" of cracks.

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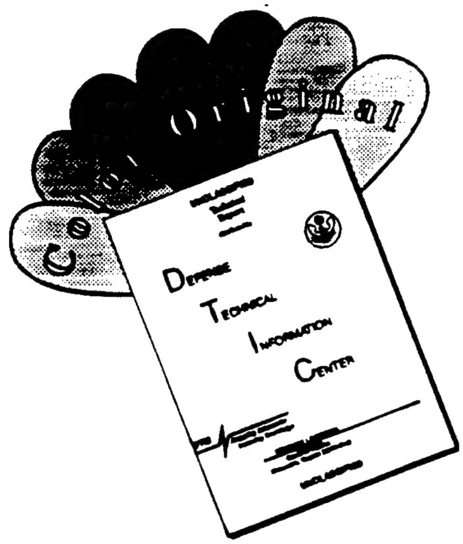

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1. Objectives

Goal: The twofold objectives of this project were (i) modeling and analysis of problems in ceramic material fabrication and (ii) the development of adaptive and parallel techniques to automate the solution of these problems.

Problems involved (i) fabrication of ceramic-matrix composites by vapor infiltration and deposition processes, (ii) the coating of ceramic fibers by vapor deposition, and (iii) estimates of the longevity of ceramic composites when subject to oxidation at elevated temperatures. Although specific processing problems were addressed, the models and parallel adaptive software have a much wider range of applicability. The adaptive techniques combine mesh refinement and coarsening (h-refinement), method-order variation (p-refinement), and mesh motion (r-refinement) in both space and time. The software executes on serial and parallel computers and operates under the Message Passing Interface (MPI). It is, thus, portable and efficient.

Highlights of our findings are presented in Section 2 and more detailed descriptions follow in Section 3. Supported personnel are listed in Section 4, Publications appear in Section 5, and presentations, interactions, and transitions appear in Section 6.

2. Significant Accomplishments and Findings

2.1. Parallel Adaptive Computation

Adaptive computation provides the most effective way of generating reliable, efficient, and robust solutions of large-scale problems involving partial differential equations. Beginning with a trial solution generated on a coarse mesh with a low-order method, an adaptive computation appraises the accuracy of a solution, enriches the solution where needed by combinations of h-, p-, and r-refinement, and recursively generates solutions until prescribed accuracy requirements have been satisfied. Error estimates control adaptive enrichment and provide a requisite measure of solution accuracy. Without such error estimates, computations must either be repeated with, e.g., finer meshes or solution accuracy must be inferred using independent knowledge of the anticipated solution. The former approach is inefficient and impractical with truly demanding problems while the latter approach provides qualitative information at best and is becoming less-and-less possible with the complexities of modern engineering systems. Error estimates obtained by order embedding (p-refinement) are asymptotically correct and have expenses ranging from one-third to one-half of the solution cost. Combinations of h- and p-refinement are remarkably efficient and may have exponential convergence rates.

Parallel computation is essential for demanding multi-dimensional, nonlinear problems. However, developing parallel adaptive software is quite a challenge. Adaptive procedures use nonuniform structures and complex heuristics to achieve efficiencies. These are difficult to parallelize using standard constructs. Load balancing must be dynamic, since adaptive enrichment will upset a balanced computation

We have developed a parallel adaptive computational framework for solving three-dimensional transient and steady partial differential equations by finite element and finite volume schemes. The software has overcome many of the cited difficulties and contains several novel and innovative features including:

- Automatic three-dimensional grid generation by recursive octree decomposition with an interfaces to several CAD systems [11].*
- Adaptive h-, p-, and r-refinement procedures [11-13]. (Adaptive p-refinement is not yet operational in three dimensions.)
- A mesh database for the efficient storage of information associated with high-order finite element computation [11].
- Dynamic load balancing by iterative tree [3-4, 7-8, 10-13], inertial bisection [11], and octree bisection [7] procedures.
- A parallel mesh database to handle the migration of data and communications between processors [4, 8, 11].
- Adaptive h- and p-refinement procedures for temporal integration that include backward-difference and singly implicit Runge-Kutta methods.
- Computational linear algebra routines that interface with the mesh and parallel mesh databases.
- Visualization software using Data Explorer.

This is the first adaptive system containing these capabilities. The framework uses the object-oriented methodology to ease development and maintenance and, as noted, the MPI for portability. Scalability has been verified by extensive computation on fluid flow [12] and crystal growth problems. Although this grant has ended, work on this effort is continuing as part of an AFOSR MURI grant. Additional development will enhance the time integration and linear algebraic procedures, improve the migration strategies, and optimize the hp- and hpr-refinement techniques. The final framework will simplify the development of new finite element applications. Many will only require software for the generation of element stiffness matrices and preconditioners.

2.2. Composite Materials Fabrication

Working with colleagues at Rensselaer's Materials Science and Engineering Department, the Air Force's Wright Laboratories, Centric Engineering, and Dupont Lanxide, we modeled processes for manufacturing ceramic matrix composites, coating ceramic fibers, and oxidizing ceramic composites at elevated temperatures.

Ceramic composites offer several advantages relative to homogeneous materials when used in high-temperature applications such as heat exchangers, heat engine components, and aerodynamic surfaces exposed to hypersonic flows. Their fabrication by a variety of techniques (e.g., plasma spraying, sintering, or chemical vapor infiltration) remains difficult. Processing times are long and production costs are high. Mathematical modeling and computational experimentation are identifying improved or optimal materials and fabrication techniques for military and civil applications.

As noted, ceramic composities operate in hostile environments and are subject to chemical, thermal, and mechanical attack. Bonds between fibers and the matrix can fail. Oxidizing reactions can weaken or destroy both fiber and matrix. Fiber coatings can

* Cited references appear in Section 5.

provide better adhesion with matrix materials as well as protect fibers from chemical attack. Cracks in the matrix can destroy protective fiber and matrix coatings and expose the interior of the composite to the caustic environment. Materials may oxidize during prolonged exposure and this may seriously degrade the mechanical properties of the composite. Alternatively, volume expansion accompanying reaction may close (or "heal") the crack before substantial damage can occur. Again, mathematical modeling can illuminate these phenomena and suggest materials and strategies that limit adverse effects.

We have investigated these issues and our key findings and results follow.

- We developed a model for fabrication of ceramic composites by reactive vapor infiltration (RVI) that couples reaction with mechanical deformation. The model and adaptive software have predicted pore closing between powder grains, deformation caused by reaction, and residual stresses [6, 9, 15].

- Using the RVI model, we showed that fabrication times and excessive deformation of molybdenum-disilicide-matrix composites may be reduced by initiating the process with a mixture of 50% powdered molybdenum and 50% molybdenum disilicide. This strategy was born out experimentally and the resulting composites had excellent mechanical properties [9, 15].

- We developed a model for the coating of ceramic fibers by chemical vapor deposition (CVD). The model has capabilities to analyze transient and steady flows containing multiple species; chemical surface reactions; heating in hot- and cold-walled reactors by conduction, convection, and radiation; and geometric variation due to fiber motion and deposition [17].

- The fiber coating model has been used to study the coating of sapphire fibers with beta-alumina in hot-walled reactors. We examined critical parameters (flow rate, fiber speed, precursor injection rates, reactor temperature and pressure) and suggest strategies that minimize losses. Since the walls of the reactor are heated with the fiber, they too are coated. We developed parameter choices that minimize wall coating and process time while producing a uniform fiber coating [17].

- Researchers at the Air Force's Wright Laboratories are using our fiber coating model and software to design a control system for their experimental facility. They will use the model's predictions to create a neural-network model of the parameter space that will provide an active control strategy during processing.

- We developed a model for the oxidation of ceramic composites at elevated temperatures. The model addresses the flow of oxidants in a crack or pore and their reaction with and diffusion through surfaces to oxidize the matrix material. It has capabilities to handle an arbitrary number of chemical species, surface and bulk reactions, and fluid and solid-state diffusion. It is coupled with a mechanical deformation model to predict stress concentration and further cracking or the healing of cracks by expansion of the matrix [18].

- The model is being used to study the oxidation of silicon-carbide matrix composites by oxygen and water vapor. This work is in collaboration with Materials Scientists at Rensselaer and at Dupont Lanxide.

All models were discretized and solved by finite element methods using the adaptive and parallel framework. The teaming of this theoretical analysis with experimental

investigation enabled knowledge to obtained more rapidly than each would have alone. The theoretical studies identified parameter values that were likely to lead to improvements. These computational investigations took far less time than experimentation, which often requires several days. Experimentation, on the other hand, provided the necessary data and constitutive parameters to the mathematical model.

3. Models and Methods

3.1. Adaptive Computation

The adaptive and parallel computational framework for partial differential systems has the generic form

$$\partial_t \mathbf{m}(\mathbf{x},t,\mathbf{q}) + f(\mathbf{x},t,\mathbf{q},\nabla\mathbf{q}) = \nabla\cdot\mathbf{d}(\mathbf{x},t,\mathbf{q},\nabla\mathbf{q})$$

where $\mathbf{x}$ and t denote space and time, $\mathbf{q}(\mathbf{x},t)$ denotes the solution vector, ∂_t denotes partial differentiation with respect to t, and ∇ denotes the gradient and divergence operators. The "mass matrix" $\partial_{\mathbf{q}}\mathbf{m}$ and the "diffusion matrix" $\partial_{\nabla\mathbf{q}}\mathbf{d}$ may be singular so the system may be of mixed type. The above equations are discretized by the finite element method in space and by either singly-implicit Runge-Kutta (SIRK) methods or backward difference formulas (BDFs) in time. These combinations have been successfully used to solve problems involving fluid flow [3, 8, 10, 11, 13] and crystal growth in addition to the materials processing problems described herein. High-order finite element bases are available using hierarchical bases where polynomial representations of the solution are regarded as corrections to lower order polynomials.

Special stabilization terms are available to handle systems where reaction and/or convection dominate diffusion. This is the case with the materials fabrication problems under investigation. When not done, solutions of these systems exhibit spurious oscillations. The stabilization model used for this study was developed in collaboration with researchers at Centric Engineering. As noted, SIRK and BDF techniques are used for time integration. These may be done as a method of lines (MOL) formulation, where the method and time step are independent of the spatial location, or as a local refinement method (LRM), where different methods and time steps are used in different spatial regions. The latter alternative is being implemented in three dimensions, but its performance in two dimensions has shown it to be a very effective method. SIRKs have remarkable stability properties and efficiencies rivaling those of BDFs. They shine when used with LRMs and in evolving geometry problems.

Estimates of spatial discretization involve the comparison of solutions obtained with different order finite element approximations. Localization, made possible through superconvergence, simplifies the computation and enables estimation at the element level [5, 14]. Accuracy appraisal is used to drive the adaptive procedure, but is also important to provide assurance that the solution is being calculated correctly.

Algebraic solutions are obtained using direct methods (sparse Gaussian elimination) for smaller problems and generalized residual methods with preconditioning for larger problems. Preconditionings are difficult to generalize and currently involve multilevel and relaxation techniques.

3.2. Parallel Computation

To operate effectively in a parallel solution environment each of the components of an automated adaptive analysis system must operate in parallel and maintain computational effectiveness as the problem scales. Key to maintaining parallel performance is the inclusion of procedures that directly account for the adaptive nature of the numerical discretization, and that maintain the appropriate balance of computational work load over the processors.

Current load balancing methods involve iterative neighborhood relaxation [3-4, 7-8, 10-13], inertial bisection [11], and octree bisection [7]. All execute in dynamic environments that restore a balanced computation that was interrupted by adaptivity. The former constructs and balances load-request trees where each processor requests load from its most heavily loaded neighbor. The latter two procedures recursively bisect the mesh in directions perpendicular to its principal axis of inertia and coordinate axes, respectively. Mesh and solution data are migrated between processors by parallel sort and communication-reduction schemes [4, 11].

The framework has capabilities to support parallel hp- and hpr-refinement methodologies for multi-dimensional problems. Future versions will use object-oriented methodology to provide commonality and reuse by abstracting many operations and algorithms to allow them to be combined in various ways to produce an application. Examples of common items are time integration procedures, linear and nonlinear algebraic solution techniques, spatial integration routines, mapping procedures from physical to the parametric space of an element, and interpolations of field variables over the mesh entities (volumes, faces, edges, and vertices).

When the geometric domain evolves with the solution, its representation must be properly updated to account for appropriate smoothness requirements and surface motion. Basic tools to update smooth geometric representations as dictated by the motion of the discrete mesh representation are available; however, they are limited in their ability to effectively support irregular meshes and computational procedures. Development will be necessary to update geometric model surface representations to support remeshing or other operations needing geometric information such as curvature.

3.3. Reactive Vapor Infiltration

With Rensselaer Materials Scientists William Hillig and John Hudson, we studied RVI techniques for manufacturing ceramic composites where silicon carbide (SiC) or alumina (Al_2O_3) fibers are mixed with molybdenum (Mo) powder or a mixture of Mo and molybdenum disilicide ($MoSi_2$) and pressed into a porous preform. The preform is exposed to a silicon tetra-chloride ($SiCl_4$) and hydrogen (H_2) flow where molecular-surface reactions liberate Si which, when absorbed into the preform, reacts with the powder to form the $MoSi_2$ matrix. We developed a model of this process that accounted for the conservation of mass of the various chemical species, the diffusion of Si into the porous media, the formation of an intermediate silicide Mo_5Si_3, and the deformation of the viscous media that results from pores filling between powder grains [6, 9, 15].

When an initial Mo powder was compressed to a porosity of 45%, the siliciding reactions produced a 158% volume increase that filled pores, but was large enough to swell the material and cause cracking. We discovered that pores could be filled with essentially no additional material expansion and that production times could be cut in half

by initiating the process with a powdered mixture of 50% Mo and 50% $MoSi_2$ [9].

Some of our findings [9] are illustrated in Figure 1. At the upper left, we present a micrograph of a cut section through a partially silicided pellet. The top and right portions of this micrograph contain the desired $MoSi_2$ matrix; the left and bottom portions contains unreacted Mo; and the band running from the left edge to the bottom contains Mo_5Si_3. The hardness indentations show the increased density in the $MoSi_2$ portion of the specimen. The computed solution at a comparable time is shown at the upper right of Figure 1. The color red indicates $MoSi_2$, yellow indicates Mo_5Si_3, and blue indicates unreacted Mo powder. The computational mesh is finer near the reaction front (Mo_5Si_3) and moves inward (towards the bottom left corner) as the reaction progresses. Material distortion is apparent in mesh lines that were originally parallel to the coordinate axes. Computed results were excellent and volumes and thicknesses of the $MoSi_2$ and Mo_5Si_3 layers as functions of time differed by less than 10% [6, 9] from experimental observations.

In the lower portion of Figure 1, we display a pore between two grains of Mo powder at two times. The pore is closing as the reaction proceeds (left to right) and closes completely after approximately two seconds on the siliciding reaction. As pores close, siliciding proceeds by solid-state diffusion. This is inefficient and a method to keep the pores open is needed. This might be possible by using microwave heating.

3.4. Ceramic Fiber Coating

Researchers in Steven Le Clair's manufacturing group at Wright Laboratory have been studying the coating of continuous sapphire fibers by beta-alumina using CVD in hot-walled reactors. We formulated a model for their process using the Navier-Stokes and energy equations to model the flow of carrier gas through the reactor. Precursor species that react on heated surfaces to form the coating are passively convected by the carrier gas. The surface reaction model includes capabilities for molecular surface impingements with and without successful reactions. This system is coupled with an energy equation and thickness variation model for the fiber. The fiber may be heated by conduction, convection, and/or radiation. As noted, the Navier-Stokes equations have been stabilized by the addition of a least-squares local diffusion model that prevents spurious oscillations without introducing excessive diffusion. This latter aspect of our investigation was done in collaboration with Centric Engineering.

While experimental results at Wright Laboratories are not yet available, the model and its computational results appear to be qualitatively correct. Parameter values, within experimental range, have identified strategies that reduce wall coating while producing fibers having uniform coatings. Concentrating the precursor near the fiber and away from the hot wall provides the most substantial improvement in the efficiency of hot-walled CVD reactors. Higher reaction probabilities yield higher efficiencies, especially when the precursor enters near the fiber. Longer dwell times (the time that the precursor remains in the reactor), controlled by either the reactor length or flow rate, improve production rates but reduce efficiency.

Results in Figure 2 show the concentration of the precursor as a function of Froude number

$$Fr = \bar{U}^2/(g\bar{L})$$

where $\overline{U}$ is a reference velocity, g is the acceleration of gravity, and $\overline{L}$ is the reactor length. In each drawing, the fiber is located on the left and the wall is located on the right of the cylindrical reactor. The illustrated reactor has a cold wall with the fiber heated by resistive heating. The Reynolds number (Re), Prandtl number (Pr), and flow rate (Sc) are indicated at the bottom of the figure. Other parameters are recorded in Adjerid et al. [17]. An axisymmetric steady solution was generated using piecewise linear finite elements and adaptive h-refinement on an initial 15×30 mesh. The color red denotes a high concentration of precursor and blue denotes a low concentration. The flow enters the bottom of the reactor and exits at the top. The fiber is heated in the central portion of the reactor.

For low values of Fr, the flow circulates and less precursor exits the reactor at the top. Larger values of Fr have higher speeds and less precursor gets used for coating.

The Manufacturing Group of Wright Laboratories has been given a copy of our software and has been using it to conduct parameter studies in preparation to performing experiments. They will also use it to design a neural network that will be used to provide an active control of parameters during fiber coating.

3.5. Oxidation of Ceramic Composites

We have developed a model to study the oxidation of SiC/SiC composites in cracks. The model includes solid- and gaseous phase-reactions and viscous momentum equations; reactions at crack surfaces; and bulk and Knudsen diffusion. Reactions between seven chemical species (silicon carbide SiC, silicon dioxide SiO_2, water vapor H_2O, oxygen O_2, carbon monoxide CO, carbon dioxide CO_2, and hydrogen H_2) are tracked. The model contains features similar to the RVI and fiber coating models of the two previous sections but is more complex. Nevertheless, this similarity and the structured design of the software enabled us to implement the without excessive coding.

This study has not been completed but work is continuing and results will be reported [18]. A preliminary computation appears in Figure 3. The figure shows half of a symmetric idealized crack at the bottom penetrating a SiC matrix. Surface reactions liberate O_2 which diffuses into the matrix and oxidizes the SiC (shown in red) to form a SiO_2 layer (shown in blue). The narrow yellow band between the SiC and SiO_2 identifies the reaction zone. CO and CO_2, created by the oxidizing reaction, diffuse through the solid surface and escape through the crack. These and other gaseous effects are not shown in Figure 2.

The solid is extremely viscous at the operating temperature (1200 °C) and motion of the solid is not apparent at the recorded times. The adaptive mesh is concentrated near the reaction zone and follows the front as it progresses through the matrix.

Reactive Vapor Infiltration

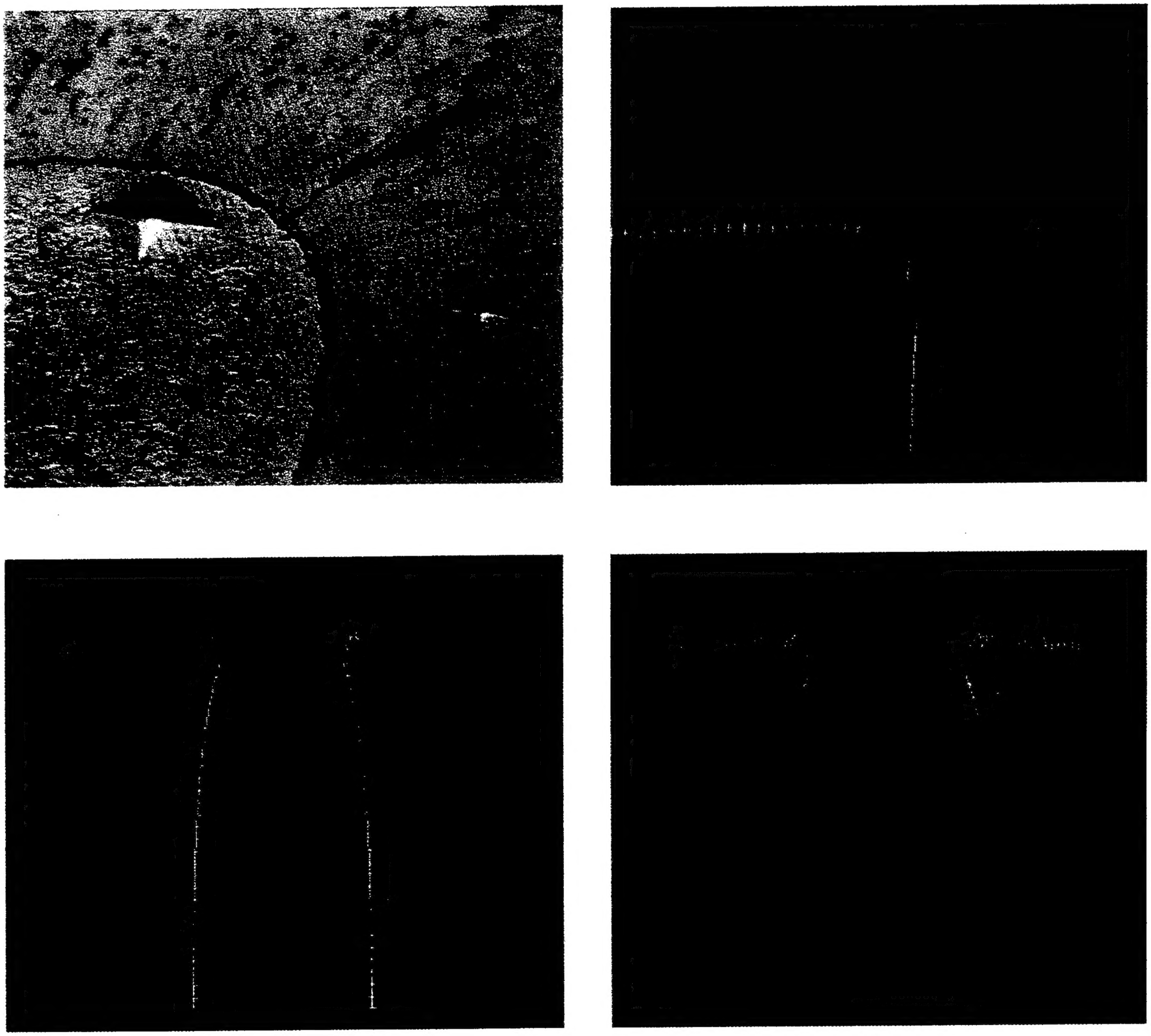
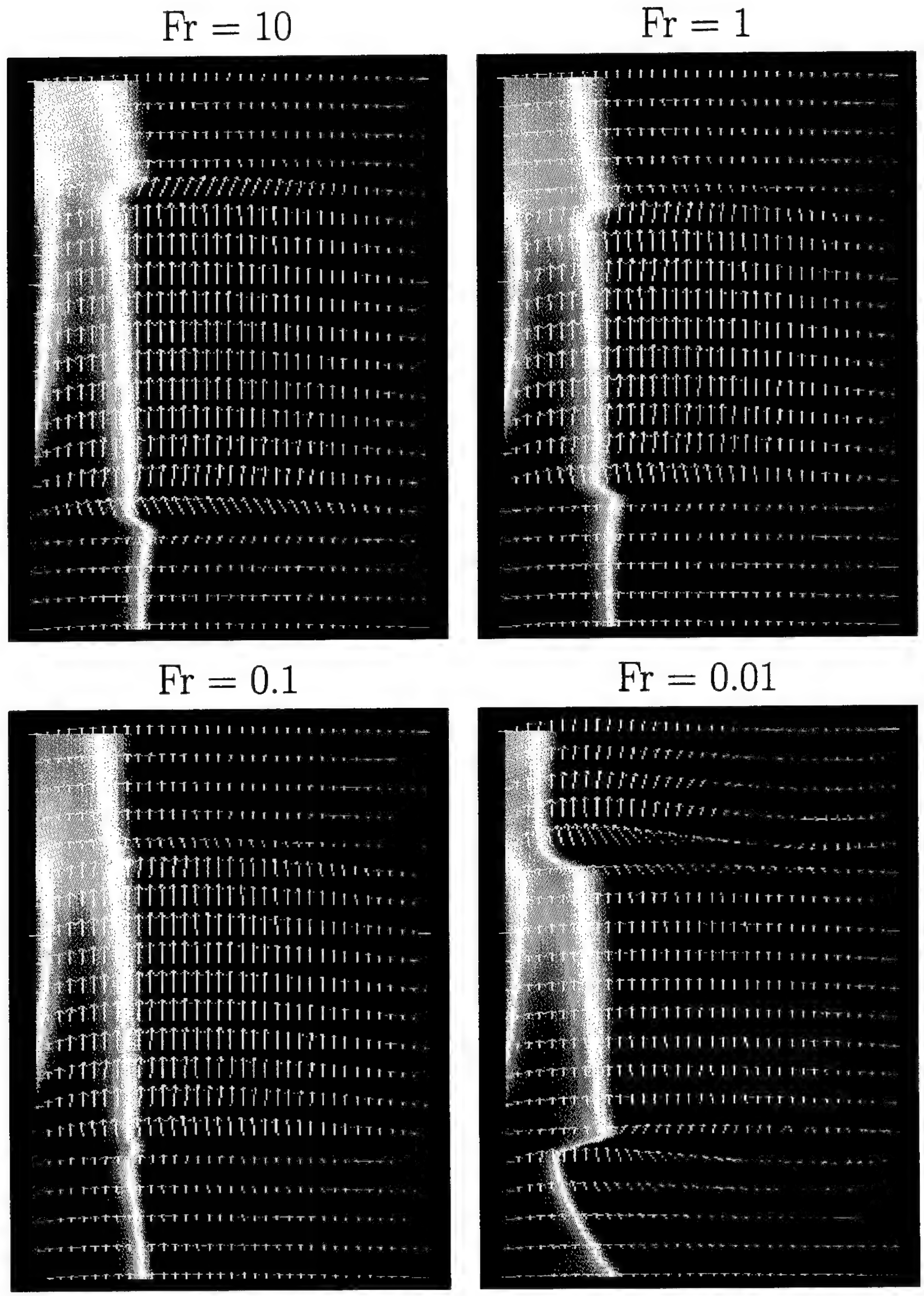


Figure 1

Figure 2.

Ceramic Fiber Coating
Flow and Precursor vs. Froude Number

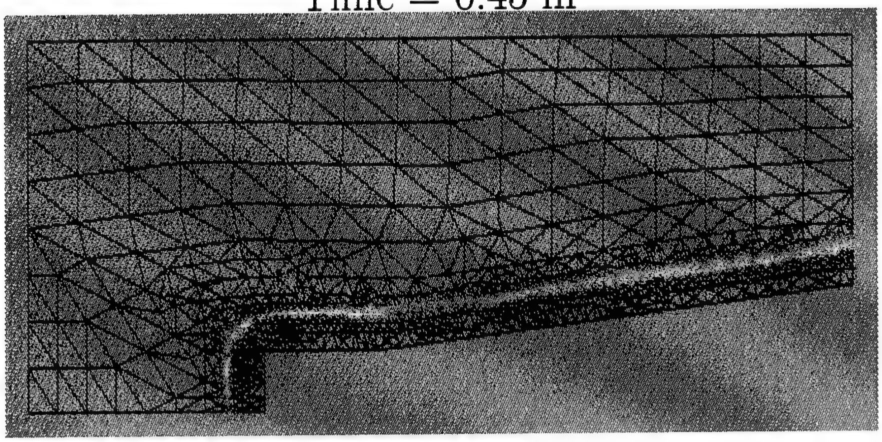


Re = 1000, Pr = 0.1, Sc = 0.0001

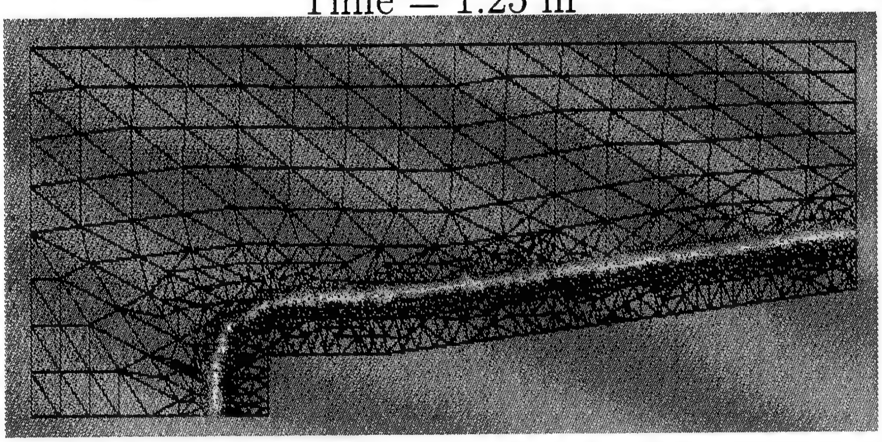
Figure 3.

Oxidation of Silicon Carbide

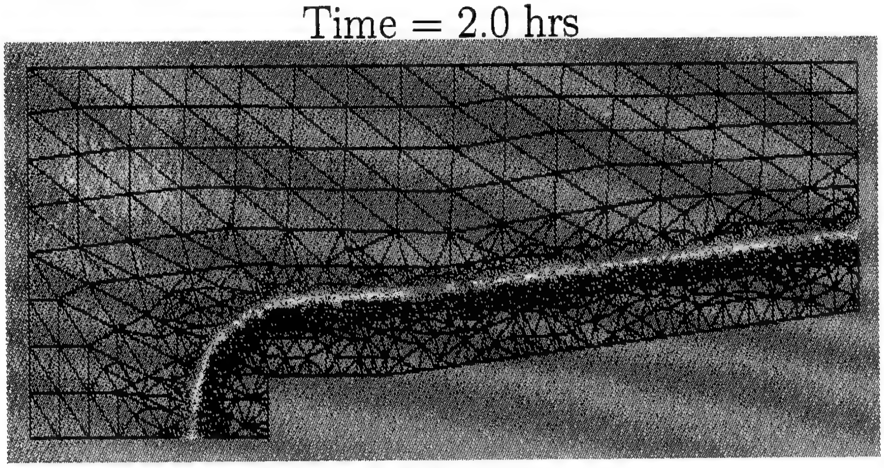
Time = 0.45 hr



Time = 1.25 hr



Time = 2.0 hrs



4. Personnel Supported

The scientists being supported by this grant are:

1. Joseph E. Flaherty, Amos Eaton Professor of Computer Science, Principal Investigator

2. Slimane Adjerid, Research Associate Professor of Computer Science, Senior Investigator

3. Mohammed Aiffa, Graduate Student, Applied Mathematics

We also interacted with Rensselaer faculty William Hillig and John Hudson of the Materials Science and Engineering Department and Mark Shephard of the Civil Engineering Department who were not supported by this grant. Hillig and Hudson conduct experiments on ceramic composite fabrication while Shephard works on mesh generation and adaptive refinement. A portion of the work reported here was in collaboration with Thomas Hughes, Robert Ferencz, and Bruce Webster of Centric Engineering who were supported (for nine months) by an AFOSR STTR (Phase 1) contract.

5. Publications

5.1. Monographs

1. K. Clark, J.E. Flaherty, and M.S. Shephard, Eds., *Appl. Numer. Maths.*, **14** (1994), Nos. 1-3, 365 pages. Special edition on *Adaptive Methods for Partial Differential Equations.*

2. I. Babuska, J.E. Flaherty, W.D. Henshaw, J.E. Hopcroft, J.E. Oliger, and T. Tezduyar, Eds., *Modeling, Mesh Generation, and Adaptive Numerical Methods for Partial Differential Equations,* The IMA Vols. in Maths. and its Applics, **75** (1995), Springer-Verlag, New York, 450 pages.

5.2. Journal Articles and Refereed Conference Proceedings

3. R. Biswas, K. Devine, and J.E. Flaherty, Parallel adaptive finite element methods for conservation laws, *Appl. Numer. Maths,* **14** (1994) 255-284.

4. C. Ozturan, H.L. deCougny, M.S. Shephard, and J.E. Flaherty, Parallel adaptive mesh refinement and redistribution on distributed memory computers, *Comp. Meths. Appl. Mech. and Engng.,* **119** (1994), 123-137.

5. S. Adjerid, M. Aiffa, and J.E. Flaherty, High-order finite element methods for singularly-perturbed elliptic and parabolic problems," *SIAM J. Appl. Math.,* **55** (1995), 520-543.

6. S. Adjerid, J.E. Flaherty, M. Shephard, Y. Wang, J. Hudson, W. Hillig, and N. Patibandla, Adaptive numerical techniques for reactive vapor infiltration, *Ceram. Engng. and Sci. Proc.,* **15** (1994), 924-931.

7. H.L. deCougny, K.D. Devine, J.E. Flaherty, R.M. Loy, C. Ozturan, and M.S. Shephard, Load balancing for the parallel adaptive solution of partial Differential equations, *Appl. Numer. Maths.,* **16** (1994), 157-182.

8. C.L. Bottasso, H.L. DeCougny, M. Dindar, J.E. Flaherty, C. Ozturan, Z. Rusak, and M.S. Shephard, Compressible aerodynamics using a parallel adaptive time-discontinuous Galerkin least-squares finite element method, AIAA Paper 94-1888, 12th AIAA Appl. Aerodyn. Conf., June 20-22, 1994, Colorado Springs.

9. S. Adjerid, J.E. Flaherty, W. Hillig, J. Hudson, and M.S. Shephard, Modeling and the adaptive solution of reactive vapor infiltration problems, *Model. and Simul. in Mat. Sci. Engng.*, **3** (1995) 737-752.

10. C.L. Bottasso, J.E. Flaherty, C. Ozturan, M.S. Shephard, B.K. Szymanski, J.D. Teresco, and L.H. Ziantz, The quality of partitions produced by an iterative load balancer, in B.K. Szymanski and B. Sinharoy, Eds., *Languages, Compilers and Run-Time Systems for Scalable Computers,* Kluwer, Boston, 1995, 265-277.

11. M.S. Shephard, J.E. Flaherty, H.L. de Cougny, C. Ozturan, C.L. Bottasso, and M.W. Beall, Parallel automated adaptive procedures for unstructured meshes, AGARD Rep. R-807, *Special Course on Parallel Computing in CFD,* AGARD, Neuilly-sur-Seine, 1995.

5.3. Manuscripts

12. K. Devine and J.E. Flaherty, Dynamic load balancing for parallel finite element methods with adaptive h- and p-refinement, 1995, submitted for publication.

13. K. Devine and J.E. Flaherty, A parallel adaptive hp-refinement finite element method with dynamic load balancing for the solution of hyperbolic conservation laws, Tech. Rep. 95-11, Dept. Comp. Sci., Rensselaer Polytech. Inst., May 1995. Also, submitted for publication.

14. S. Adjerid, B. Belguendouz, and J.E. Flaherty, A posteriori finite element error estimation for diffusion problems, SCOREC Rep. No. 9-1996, Sci. Comput. Res. Ctr., Rensselaer Polytech. Inst., Troy, 1996. Also, submitted for publication.

15. S. Adjerid, M.W. Beall, G.J. Dvorak, J. Fish, J.E. Flaherty, J. Hudson, K.-L. Shek, M.S. Shephard, and R. Wentorf, Mechanism-based design of composite Structures, submitted to IMECE, ASME, Atlanta, June 1996.

16. B.K. Szymanski, E. Deelman, J.E. Flaherty, C.D. Norton, J.D. Teresco, and L.H. Ziantz, Parallel scientific computing on the IBM SP2 at SCOREC-Rensselaer Polytechnic Institute," submitted for publication.

5.4. Manuscripts in Preparation

17. S. Adjerid, J.E. Flaherty, J. Hudson, and M.S. Shephard, Modeling and the adaptive solution of CVD processes for coating ceramic fibers, 1996, in preparation.

18. S. Adjerid, M. Aiffa, J.E. Flaherty, and J. Hudson, The oxidation of ceramic composites at elevated temperatures, 1996, in preparation.

6. Interactions and Transitions

6.1. Presentations

1. Flaherty presented an invited lecture on ''Parallel Adaptive Finite Element Computation'' at the Conf. on *Application of High Performance Computing in Bioengineering,* Pittsburg Supercomputing Center, October, 21-22, 1994, Pittsburg.

2. Flaherty presented an invited lecture ''Adaptive High-Order Computational Techniques for Singularly-Perturbed Elliptic and Parabolic Systems'' at the meeting on *Numerical Methods for Singular Perturbations,* Oberwolfach, January 22-28, 1995.

3. Flaherty presented an invited lecture ''Adaptive Computational Methods for Composite Materials Processing'' Minisymp. on ODE Methods in PDEs, SCICADE 95, Int. Conf. on Sci. Comput. and Diff. Eqns., Stanford University, Palo Alto, March 28-April 1, 1995.

4. Flaherty presented an invited lecture ''Adaptive Computational Methods for Composite Materials Processing'' at the workshop *Applied Mathematics: Methods and Applications,* Rensselaer Polytechnic Institute, Troy, March 24-25, 1995.

5. Flaherty presented a seminar ''Parallel Adaptive Load-Balancing Schemes for Three-Dimensional Conservation Laws'' at New York University, April 7, 1995, New York.

6. Adjerid presented a lecture ''Modeling and Adaptive Numerical Solution of Fiber Coating by Chemical Vapor Deposition'' at *Aeromat 95,* ASM Sixth Int. Aero. Mats. and Processes Conf., Anaheim, May 6-11, 1995.

7. Flaherty presented an invited lecture ''Adaptive Method of Lines Techniques for Parabolic Systems with Applications to Materials Processing'' *Workshop on the Method of Lines for Time Dependent Problems,* University of Kentucky, Lexington, May 31 - June 3, 1995.

8. Adjerid presented a lecture ''A Posteriori Error Estimation for Parabolic Systems'' *Workshop on the Method of Lines for Time Dependent Problems,* University of Kentucky, Lexington, May 31 - June 3, 1995.

9. Flaherty presented an invited lecture ''Adaptive Computational Methods for Composite Materials Processing'' at the symp. on *Numerical Methods for Industrial Manufacturing Processes 1: Composite Materials, Third U.S. Nat. Congr. of Comput. Mech.,* Dallas, June 12-14, 1995.

10. Adjerid presented an invited lecture ''Modeling and Adaptive Numerical Solution of Fiber Coating by Chemical Vapor Deposition'' at the symp. on *Numerical Methods for Industrial Manufacturing Processes 1: Composite Materials, Third U.S. Nat. Congr. of Comput. Mech.,* Dallas, June 12-14, 1995.

11. Flaherty presented a lecture on ''Adaptive and Parallel Computational Techniques in Materials Science,'' at the *1995 AFOSR Grantees/Contractors Meeting in Computational and Physical Mathematics,* Albuquerque, June 28-30, 1995.

12. Flaherty presented an invited lecture ''Adaptive Methods for Parabolic Partial Differential Equations with Applications to Shear Band Formation'' at *ICES 95,* Int. Conf. on Comput. Engng. Sci., Mauna Lani, July 30 - Aug. 3, 1995.

13. Flaherty presented an invited lecture ''Adaptive and Parallel Computational Techniques,'' at the IBM Symposium on Parallel Computation, *Supercomputing '95,* San Diego, December 4-8, 1995.

14. Flaherty presented a seminar on ''Adaptive and Parallel Computational Techniques with Applications in Materials Science,'' Air Products, Inc., Allentown, January 23, 1996.

15. Flaherty presented the Schiesser Lecture in Interdisciplinary Science and Engineering on ''Adaptive Method of Lines Techniques for Parabolic Systems with Applications to Materials Processing,'' Lehigh University, January, 24, 1996.

16. Flaherty presented a seminar on ''Adaptive and Parallel Computational Techniques for Partial Differential Equations,'' U.S. Army High Performance Computation Center, University of Minnesota, February 8 1996.

17. Flaherty presented a seminar on ''Adaptive and Parallel Computational Techniques for Partial Differential Equations,'' Theory Center, Cornell University, March 4, 1996.

18. Flaherty presented a seminar on ''Adaptive and Parallel Computational Techniques for Partial Differential Equations,'' Department of Applied Mathematics, Brown University, March 8, 1996.

19. Flaherty gave a talk on ''Adaptive and Parallel Computation for Materials Processing'' at the *AFOSR Grantees and Contractors' Meeting: Computational and Physical Mathematics,* Wright Laboratories, Wright Patterson Air Force Base, June 24-26, 1996.

20. Flaherty gave a keynote lecture on ''High-Order Adaptive Computational Methods With Applications in Materials Science'' at the *Conference on Grid Adaptation in Computational PDEs: Theory and Applications,* University of Edinburgh, Edinburgh, July 1-5, 1996.

6.2. Advisory Functions to Laboratories and Agencies

1. Adjerid, Flaherty, and Hudson, visited the Manufacturing group at Wright Laboratories, Wright-Patterson Air Force Base, on December 12, 1994. We met with Steven Le Clair, James Malas, John Busbee, et al. and discussed our research on the coating of sapphire fibers in relation to their experimental work on the same topic. Bruce Webster of Centric Engineering was also in attendance.

2. Adjerid and Flaherty collaborated with Robert Ferencz, Thomas Hughes, and Bruce Webster of Centric Engineering on modeling and the numerical solution of fiber coating processes. Ferencz visited Rensselaer on July 12-14, 1995 and Flaherty visited Centric on March 30 and July 28, 1995.

3. Adjerid and Flaherty met with John Garnier of Du Pont Lanxide to discuss our mutual interests in processes to coat ceramic fibers, June 1, 1995. Lanxide is providing silicon carbide/silicon carbide composite samples to Rensselaer researchers for mechanical testing. These composites contain coated fiber tows and their data could provide an excellent platform for testing our models and software.

4. Richard K. Everett of the Naval Research Laboratory has expressed an interest in collaborating with us on an investigation involving the reaction and diffusion between nickel and aluminum films in multilayers. Adjerid and Flaherty met with Everett on June 1, 1995 for an initial discussion of this possibility.

5. Flaherty visited Karen Devine, Andrew Salinger, and John Shadid of Sandia National Laboratories, June 28, 1995 to discuss our parallel adaptive software for solving CVD problems.

6. Adjerid and Flaherty visited John Jones of Wright Laboratories on June 24, 1996 and discussed our research on fiber coating.

6.3. Transitions

1. Adjerid and Flaherty (in collaboration with Hudson and Shephard of Rensselaer and Robert Ferencz, Thomas Hughes, Bruce Webster of Centric Engineering) developed a mathematical model and computer software for analyzing axisymmetric fiber coating processes by CVD. John Jones of Wright Laboratories has a copy of this software and has been using it for parameter studies and to create a neural network model of the parameter space that will be used to control their experiments on the coating of sapphire fibers.

2. Our fiber-coating model and adaptive software will be encorporated into Centric Engineering's SPECTRUM finite element software for solving stress and fluid-flow problems.